Full-Scale Computational Study Of Electrophoretic Systems

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Computational Fluid Dynamics (CFD) has been increasingly used in recent years during design and implementation of electrophoretic devices for biological/chemical sensing applications. This requires a thorough understanding of fundamental bio-electrochemical processes that commonly occur in these systems. In this regard, CFD can provide insight into the interactions between various physical processes and help in design optimization studies. This paper is focussed on our current research effort [1,2] devoted to developing a multidisciplinary simulation environment in CFD-ACE+ [4] (simulation software) for biomicrosystem analysis.

For accurate modeling of bio-electrochemical processes, an implicit finite-volume approach has been developed [3,4] to solve the governing equations for electrophoresis and electroosmosis. Besides, biological systems consist of buffers and proteins, and modeling the ionization equilibrium is critical to satisfy electroneutrality. The simulation tool solves a set of partial differential equations expressing the conservation of mass, momentum and electric current while satisfying electroneutrality via ionization equilibria. This is done in a sequential fashion until convergence in solution is achieved.

In this work, a generalized two-step dissociation-recombination [5] model is implemented. Results from the multidimensional simulation are validated against the experimental data of Mosher et. al [6]. The model is applied to simulate real world systems such as capillary electrophoresis in a microchannel, isoelectric focussing involving separation of proteins under stable pH gradient, moving boundary electrophoresis and isotachophoresis. It will be shown that the numerical model is robust enough to predict the shape and structure, and diffusion of the analytes driven in an electric field.

References

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